

chain nodes :

7 8 9 10 11 12 13 14 15 18 19 20 21 22

ring nodes :

1 2 3 4 5 6

chain bonds :

5-7 6-18 7-8 7-9 9-10 10-11 11-12 11-13 14-15 18-22 19-20 19-22 20-21

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6

exact/norm bonds :

7-8 7-9 9-10 11-12 11-13 14-15 18-22 19-20 19-22 20-21

exact bonds :

5-7 6-18 10-11

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6

isolated ring systems :

containing 1 :

G1:H,[\*1]

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS8:CLASS9:CLASS10:CLASS11:CLASS  
12:CLASS13:CLASS14:CLASS15:CLASS18:CLASS19:CLASS20:CLASS21:Atom 22:CLASS

Generic attributes :

21:

Saturation : Unsaturated

Number of Carbon Atoms : 7 or more

Type of Ring System : Polycyclic

Element Count :

Node 21: Limited

N,N1

O,O0

S,S0

10/690400

=>

Uploading C:\Documents and Settings\EBernhardt\My  
Documents\Stnexp\Queries\10690400-7.str



chain nodes :

7 8 9 10 11 12 13 14 15 18 19 20 21 22

ring nodes :

1 2 3 4 5 6

chain bonds :

5-7 6-18 7-8 7-9 9-10 10-11 11-12 11-13 14-15 18-22 19-20 19-22 20-21

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6

exact/norm bonds :

7-8 7-9 9-10 11-12 11-13 14-15 18-22 19-20 19-22 20-21

exact bonds :

5-7 6-18 10-11

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6

isolated ring systems :

containing 1 :

G1:H, [\*1]

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS

11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 18:CLASS 19:CLASS 20:CLASS

21:Atom 22:CLASS

Generic attributes :

21:

10/690400

Saturation : Unsaturated  
Number of Carbon Atoms : 7 or more  
Type of Ring System : Polycyclic

Element Count :  
Node 21: Limited  
N,N1  
O,O0  
S,S0

L1 STRUCTURE UPLOADED

=> s l1

SAMPLE SEARCH INITIATED 13:51:31 FILE 'REGISTRY'  
SAMPLE SCREEN SEARCH COMPLETED - 2574 TO ITERATE

77.7% PROCESSED 2000 ITERATIONS 0 ANSWERS  
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)  
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*  
PROJECTED ITERATIONS: 48437 TO 54523  
PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1

=> s l1 sss full

FULL SEARCH INITIATED 13:51:40 FILE 'REGISTRY'  
FULL SCREEN SEARCH COMPLETED - 50851 TO ITERATE

100.0% PROCESSED 50851 ITERATIONS 4 ANSWERS  
SEARCH TIME: 00.00.02

L3 4 SEA SSS FUL L1

=> file caplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	172.55	172.76

FILE 'CAPLUS' ENTERED AT 13:51:48 ON 29 MAY 2007  
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17:

Saturation : Unsaturated

Number of Carbon Atoms : less than 7

Element Count :

Node 17: Limited

N,N0-1

O,00

S,S0

10/690400

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FILE COVERS 1907 - 29 May 2007 VOL 146 ISS 23  
FILE LAST UPDATED: 28 May 2007 (20070528/ED)

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They are available for your review at:

<http://www.cas.org/infopolicy.html>

=> s l3

L4 3 L3

=> d l4 1-3 bib abs hitstr

L4 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2007 ACS on STN

AN 1999:764022 CAPLUS

DN 132:3323

TI Preparation of tetrahydroisoquinolinylnicotinic acid amides and related compounds as inhibitors of cysteine proteases.

IN Lubisch, Wilfried; Moller, Achim; Treiber, Hans-Jorg; Knopp, Monika

PA BASF Aktiengesellschaft, Germany

SO PCT Int. Appl., 57 pp.

CODEN: PIXXD2

DT Patent

LA German

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9961423	A1	19991202	WO 1999-EP3549	19990525
	W: AL, AU, BG, BR, BY, CA, CN, CZ, GE, HU, ID, IL, IN, JP, KR, KZ, LT, LV, MK, MX, NO, NZ, PL, RO, RU, SG, SI, SK, TR, UA, US, ZA, AM, AZ, KG, MD, TJ, TM				
	RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				

CA 2333008	A1	19991202	CA 1999-2333008	19990525
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AU 9945003	A	19991213	AU 1999-45003	19990525
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BR 9910701	A	20010130	BR 1999-10701	19990525
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EP 1080074	A1	20010307	EP 1999-927749	19990525
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EP 1080074	B1	20061108		
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R: AT, BE, CH, DE, ES, FR, GB, IT, LI, NL, SE, FI				
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HU 200102146	A2	20011128	HU 2001-2146	19990525
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JP 2002516311	T	20020604	JP 2000-550829	19990525
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AT 344794	T	20061115	AT 1999-927749	19990525
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EP 1757584	A1	20070228	EP 2006-23149	19990525
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R: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE, AL, LT, LV, MK, RO, SI				
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US 6482832	B1	20021119	US 2000-700453	20001115
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NO 2000005929	A	20001123	NO 2000-5929	20001123
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ZA 2000007757	A	20020121	ZA 2000-7757	20001221
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PRAI DE 1998-19823245	A	19980525		
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EP 1999-927749	A3	19990525		
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WO 1999-EP3549	W	19990525		
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OS MARPAT 132:3323

AB AB(R1)nCONHCHR2COR3 [A = (substituted) tetrahydro(iso)quinolinyl, dihydro(iso)indolyl; B = Ph, naphthyl, pyridyl, pyrimidinyl, quinolyl, thienyl, furyl, etc.; R1 = H, alkyl, alkoxy, alkenyl, alkynyl, alkylphenyl, OH, Cl, F, Br, iodo, etc.; n = 0-2; R2 = (substituted) alkyl; R3 = H, CO2R5, COZ; Z = (substituted) amino, piperazinyl, pyrrolidinyl, piperidinyl; R5 = (substituted) alkyl], were prepared Thus, Et

2-chloronicotinate, 1,2,3,4-tetrahydroisoquinoline hydrochloride, and K<sub>2</sub>CO<sub>3</sub> were heated in DMF at 110° to give 87% Et 2-(1,2,3,4-tetrahydroisoquinolin-2-yl)nicotinate. This was saponified with aqueous NaOH in EtOH (81%) and the product was stirred with 3-amino-2-hydroxy-4-phenylbutyramide hydrochloride, Et<sub>3</sub>N, 1-hydroxybenzotriazole, and N'-3-dimethylaminopropyl-N-ethylcarbodiimide to give 85% 2-(1,2,3,4-tetrahydroisoquinolin-2-yl)nicotinic acid [N-(1-carbamoyl-1-hydroxy-3-phenylpropan-2-yl)]amide. The latter was stirred with pyridine.SO<sub>3</sub> in Me<sub>2</sub>SO to give 31% 2-(1,2,3,4-tetrahydroisoquinolin-2-yl)nicotinic acid [N-(1-carbamoyl-1-oxo-3-phenylpropan-2-yl)]amide.

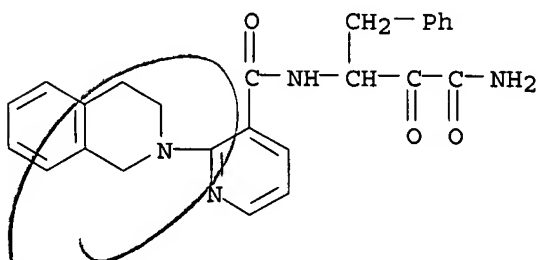
IT 247056-67-3P 247056-68-4P 250739-05-0P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of tetrahydroisoquinolinylnicotinic acid amides and related compds. as inhibitors of cysteine proteases)

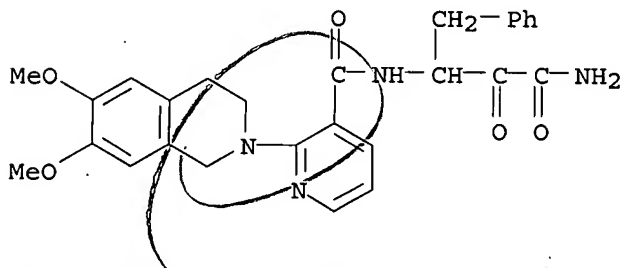
RN 247056-67-3 CAPLUS

CN 3-Pyridinecarboxamide, N-[3-amino-2,3-dioxo-1-(phenylmethyl)propyl]-2-(3,4-dihydro-2(1H)-isoquinolinylnyl)- (9CI) (CA INDEX NAME)



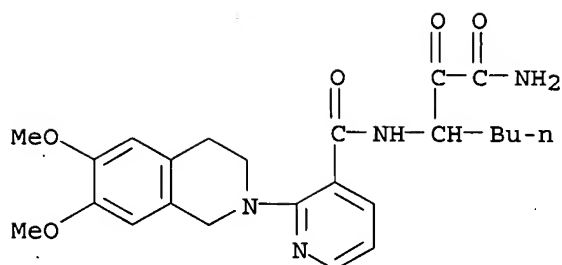
RN 247056-68-4 CAPLUS

CN 3-Pyridinecarboxamide, N-[3-amino-2,3-dioxo-1-(phenylmethyl)propyl]-2-(3,4-dihydro-6,7-dimethoxy-2(1H)-isoquinolinylnyl)- (9CI) (CA INDEX NAME)



RN 250739-05-0 CAPLUS

CN 3-Pyridinecarboxamide, N-[1-(aminooxoacetyl)pentyl]-2-(3,4-dihydro-6,7-dimethoxy-2(1H)-isoquinolinylnyl)- (9CI) (CA INDEX NAME)

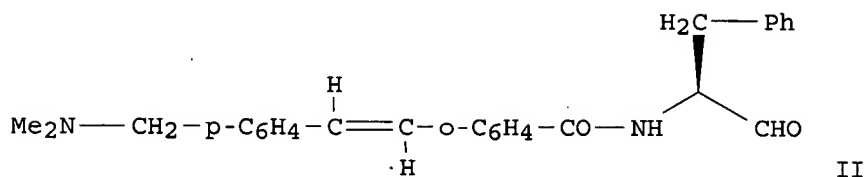
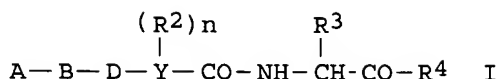


RE.CNT 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2007 ACS on STN  
AN 1999:691085 CAPLUS  
DN 131:310835  
TI Preparation of cysteine protease inhibitors for therapeutic use  
IN Lubisch, Wilfried; Moller, Achim; Treiber, Hans-Jorg; Knopp, Monika  
PA BASF Aktiengesellschaft, Germany  
SO PCT Int. Appl., 52 pp.  
CODEN: PIXXD2  
DT Patent  
LA German  
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9954310	A2	19991028	WO 1999-EP2633	19990420
	WO 9954310	A3	20000217		
	W: AL, AU, BG, BR, BY, CA, CN, CZ, GE, HR, HU, ID, IL, IN, JP, KR, KZ, LT, LV, MK, MX, NO, NZ, PL, RO, RU, SG, SI, SK, TR, UA, US, ZA, AM, AZ, KG, MD, TJ, TM				
	RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
	CA 2328396	A1	19991028	CA 1999-2328396	19990420
	AU 9939276	A	19991108	AU 1999-39276	19990420
	BR 9909774	A	20001219	BR 1999-9774	19990420
	EP 1073641	A2	20010207	EP 1999-922108	19990420
	EP 1073641	B1	20040414		
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, SI, FI, RO				
	TR 200003068	T2	20010321	TR 2000-200003068	19990420
	HU 200102732	A2	20011228	HU 2001-2732	19990420
	JP 2002512231	T	20020423	JP 2000-544649	19990420
	AT 264310	T	20040415	AT 1999-922108	19990420
	ES 2220061	T3	20041201	ES 1999-922108	19990420
	US 6753327	B1	20040622	US 2000-673089	20001011
	BG 104873	A	20010731	BG 2000-104873	20001017
	NO 2000005263	A	20001019	NO 2000-5263	20001019
	IN 2000CN00655	A	20050304	IN 2000-CN655	20001113
	HR 2000000787	A1	20010831	HR 2000-787	20001117
	ZA 2000006719	A	20020815	ZA 2000-6719	20001117
	US 2004082569	A1	20040429	US 2003-690400	20031020
PRAI	DE 1998-19818615	A	19980420		
	WO 1999-EP2633	W	19990420		
	US 2000-673089	A3	20001011		
OS	MARPAT 131:310835				
GI					





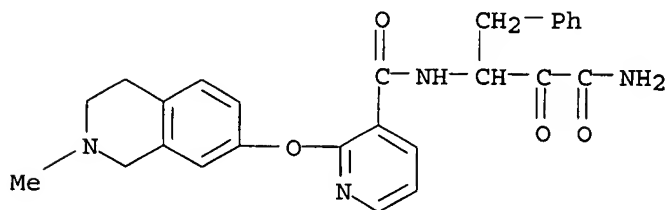
AB The invention relates to cysteine protease inhibitors of the general formula [(I); A = -(CH<sub>2</sub>)<sub>p</sub>-R<sub>1</sub>; R<sub>1</sub> = pyrrolidine, morpholine, piperidine, -NR<sub>5</sub>R<sub>6</sub>, (N-substituted)piperazine; R<sub>5</sub>, R<sub>6</sub> = independently H, alkyl, cyclohexyl, cyclopentyl, (CH<sub>2</sub>)<sub>n</sub>Ph, where Ph may be R<sub>6</sub>-substituted; p = 1-2; B = (substituted) Ph, pyridyl, pyrimidyl or pyridazyl; D = bond, -(CH<sub>2</sub>)<sub>m</sub>-, -CH:CH-, -C.tplbond.C-; R<sub>2</sub> = Cl, Br, F, alkyl, NHCO alkyl, NHSO<sub>2</sub> alkyl, NO<sub>2</sub>, -O-alkyl or NH<sub>2</sub>; R<sub>3</sub> = alkyl which can carry a (substituted) Ph ring, indolyl ring or cyclohexyl ring; Y = Ph, pyridine, pyrimidine or pyrazine; R<sub>4</sub> = H, COOR<sub>9</sub> or CO-Z, where Z = NR<sub>10</sub>R<sub>11</sub>; R<sub>9</sub>, R<sub>10</sub>, R<sub>11</sub> = (independently) H, (unsubstituted) (unbranched) alkyl; n = 0-2 and m = 0-4]. Thus, Et 2-bromo-benzoate and dimethyl(4-vinylbenzyl)amine were reacted, de-esterified, and the free acid intermediate reacted with (S)-phenylalaninol to give an intermediate which was reduced to give aldehyde (II) in 88% yield. Title compds. showed good results as inhibitors of calpain I and II or cathepsin B in a variety of in vivo and in vitro tests (no data given).

IT 247219-18-7P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(preparation of as cysteine protease inhibitors for therapeutic use)

RN 247219-18-7 CAPLUS

CN 3-Pyridinecarboxamide, N-[3-amino-2,3-dioxo-1-(phenylmethyl)propyl]-2-[(1,2,3,4-tetrahydro-2-methyl-7-isoquinolinyl)oxy]- (9CI) (CA INDEX NAME)



L4 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2007 ACS on STN

AN 1999:684297 CAPLUS

DN 131:299438

TI New substituted heterocyclic amides, their preparation and application

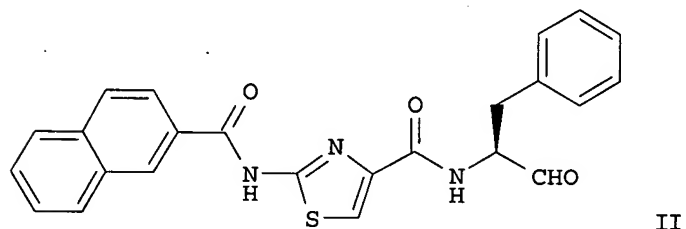
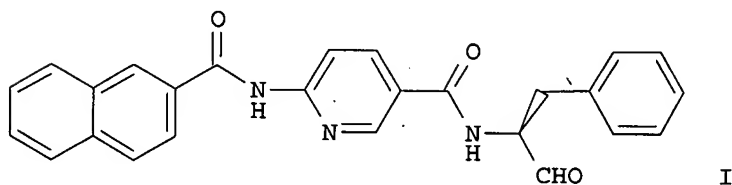
IN Lubisch, Wilfried; Moeller, Achim; Treiber, Hans-Joerg; Knopp, Monika

PA BASF A.-G., Germany

SO Ger. Offen., 36 pp.

CODEN: GWXXBX  
 DT Patent  
 LA German  
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	DE 19817459	A1	19991021	DE 1998-19817459	19980420
	CA 2328438	A1	19991028	CA 1999-2328438	19990419
	WO 9954304	A1	19991028	WO 1999-EP2611	19990419
	W: AL, AU, BG, BR, BY, CA, CN, CZ, GE, HR, HU, ID, IL, IN, JP, KR, KZ, LT, LV, MK, MX, NO, NZ, PL, RO, RU, SG, SI, SK, TR, UA, US, ZA, AM, AZ, KG, MD, TJ, TM				
	RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
	AU 9939271	A	19991108	AU 1999-39271	19990419
	BR 9909772	A	20001219	BR 1999-9772	19990419
	EP 1073638	A1	20010207	EP 1999-922102	19990419
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, SI, FI, RO				
	TR 200003056	T2	20010221	TR 2000-200003056	19990419
	HU 200101688	A2	20011128	HU 2001-1688	19990419
	JP 2002512228	T	20020423	JP 2000-544645	19990419
	BG 104831	A	20010531	BG 2000-104831	20001010
	US 6630493	B1	20031007	US 2000-673087	20001011
	NO 2000005264	A	20001019	NO 2000-5264	20001019
	HR 2000000786	A1	20010831	HR 2000-786	20001117
	ZA 2000006718	A	20011119	ZA 2000-6718	20001117
	US 2004097508	A1	20040520	US 2003-601356	20030623
PRAI	DE 1998-19817459	A	19980420		
	WO 1999-EP2611	W	19990419		
	US 2000-673087	A3	20001011		
OS	MARPAT 131:299438				
GI					



AB Heterocyclic amides such as I and II were prepared as inhibitors of enzymes, e.g., calpains and cathepsin B. Thus, II was prepared in 4 steps starting from Et 2-amino-4-thiazolecarboxylate and 2-naphthoyl chloride.

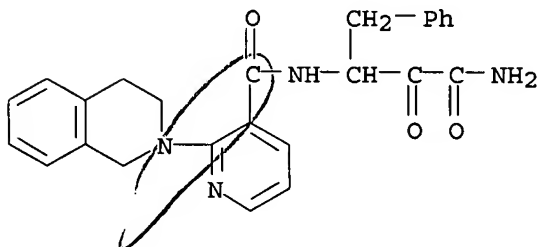
IT 247056-67-3P 247056-68-4P

10/690400

RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(heterocyclic amides as enzyme inhibitors)

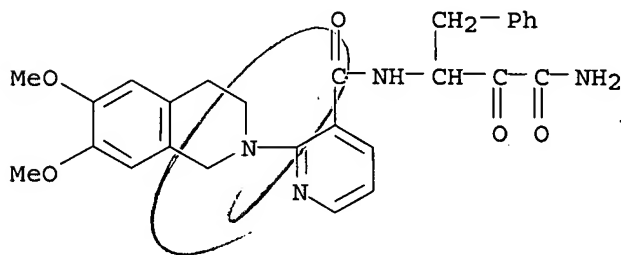
RN 247056-67-3 CAPLUS

CN 3-Pyridinecarboxamide, N-[3-amino-2,3-dioxo-1-(phenylmethyl)propyl]-2-(3,4-dihydro-2(1H)-isoquinolinyl)- (9CI) (CA INDEX NAME)



RN 247056-68-4 CAPLUS

CN 3-Pyridinecarboxamide, N-[3-amino-2,3-dioxo-1-(phenylmethyl)propyl]-2-(3,4-dihydro-6,7-dimethoxy-2(1H)-isoquinolinyl)- (9CI) (CA INDEX NAME)



=> file caold

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
18.63	191.39

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION
-2.34	-2.34

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FILE COVERS 1907-1966

FILE LAST UPDATED: 01 May 1997 (19970501/UP)

This file contains CAS Registry Numbers for easy and accurate substance identification. Title keywords, authors, patent assignees, and patent information, e.g., patent numbers, are now searchable from 1907-1966. TIFF images of CA abstracts printed between 1907-1966 are available in the PAGE display formats.

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10/690400

This file supports REGISTRY for direct browsing and searching of all substance data from the REGISTRY file. Enter HELP FIRST for more information.

=> s l3

L5                    0 L3

=> log h

COST IN U.S. DOLLARS

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ENTRY	SESSION
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FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION
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CA SUBSCRIBER PRICE

SESSION WILL BE HELD FOR 120 MINUTES

STN INTERNATIONAL SESSION SUSPENDED AT 13:55:36 ON 29 MAY 2007